

STRUCTURE ACTIVITY TEAM REPORT ver. 04/98

Case #: L-01-0546

DCN:

SAT Date: 9/28/01

SAT Chair: V. Nabholz

Submitter: Seppic, Inc.

Chemical Name:

D-Glucopyranose, homopolymer, 2-ethylhexyl glycosides

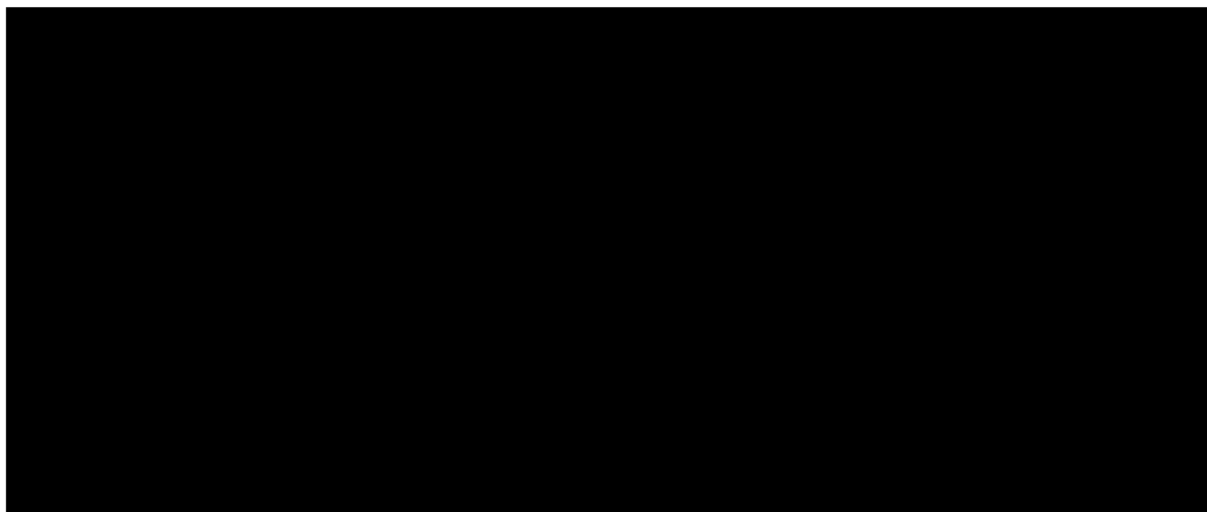
CAS RN:

None

Trade Name:

Simulsol AS48

Structure



Molecular Formula:

Molecular Wt.

WT%<500:

WT%<1000:

MP:

BP:

439

Eq. Wt:

H2O Sol (g/L):

17.1 g/L,

☒ V.P.

<0.000001

Max. Prod. Volume (kg/yr):

Physical State:

Liquid (est)

USE:

Wetting agent for use in water-based drilling muds. The alkylpolyglucoside is less toxic to algae, invertebrates and fish than the longer chain alkylpolyglucosides (C12-14), a C12 ethylglucoside monoester and a linear C12-15 alcohol ethoxylate. No references found.

Related Case Numbers	Case Role	Related Case Numbers	Case Role
Focus	Date: OCT 4 2001	Results: GRANT	



60020000078

STRUCTURE ACTIVITY TEAM REPORT 28 September 2001

CASE NUMBER: L01-0546

RELATED CASES:

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN: HEALTH ECOTOX

LEVEL: 1-2 2

KEYWORDS: AQUATOX-A,C, LUNG, IRR-E

SUMMARY OF ASSESSMENT:

FATE:
liquid with mp < 20 °C (P)
log Kow = 1.1 for monomer (SRC);
S = 17 g/L at 20 °C (P) or dispersible (P), soluble (MSDS);
vp < 1.0E-6 mm Hg or torr at 25 °C (P);
bp = 440 °C (P);
H < 1.0E-8 (P);
log Koc = 1.0 (P);
log fish BCF = 0.13 (P);
POTW removal = 90 to 99% via biodegradation;
time for complete ultimate aerobic biodegradation = days to weeks;
sorption to soils and sediments = low;
PBT Potential: P1B1T1
*CEB FATE: migration to ground water = negligible to slow;

HEALTH: Absorption poor thru skin based on analogs; good thru lungs based on analogs; and moderate thru GI tract with digestion based on analogs;
expect digestion of the glucose in the GI tract;

concern for lung toxicity if inhaled and delayed irritation to eyes based on nonionic surfactant-alkyl ethoxylate analogs;

low-moderate concern for toxicity;

*CEB HEALTH: Exposures to humans: inhalation;

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50	=>	40.0	P
daphnid 48-h LC50	=>	40.0	P
green algal 96-h EC50	=>	40.0	P
fish chronic value	=>	8.0	P
daphnid ChV	=>	8.0	P
algal ChV	=>	10.0	P

Predictions are based on SARs for nonionic surfactants-alkylethoxylates; SAR chemical class = surfactant-nonionic-alkylethoxylate; log Kow of the hydrophile

(one glucose) = the log Kow for [REDACTED] [REDACTED] [REDACTED] [REDACTED] [REDACTED]
[REDACTED]; pH7; effective concentrations based on 100%
active ingredients and mean measured concentrations; hardness
<180.0 mg/L as CaCO3; and TOC <2.0 mg/L;
moderate concern for toxicity;
assessment factor = 10.0
concern concentration = 0.800
*CEB ECOTOX: All releases to water;

SAT Co-chairperson: Vince Nabholz, 260-1271

BIOLOGICAL TEST INFORMATION				
Case Number: L-01-0546	Date Received: 9-17-01	Rev. Init: ker	OECD Status: incomplete	Page: 1 of 1
Comments: A journal article was enclosed to depict biodegradability, though no study was performed.				
Other Data:	<input type="checkbox"/> Ecotox	<input type="checkbox"/> Fate	<input checked="" type="checkbox"/> Water solubility/Log P soluble, MSDS, p17	%ai

NCSAB SAT REPORT				CBI? (Y/N):	
PMN: L-01-0546		CAS RN: None			
Chemical Name: D-Glucopyranose, homopolymer, 2-ethylhexyl glycosides				Analog:	
				Production Volume: [REDACTED]	
Structure:					
[REDACTED]					
Use: Wetting agent for use in water-based drilling muds. The [REDACTED] alkylpolyglucoside is less toxic to algae, invertebrates and fish than the longer chain alkylpolyglucosides (C12-14), a C12 ethylglucoside monoester and a linear C12-15 alcohol ethoxylate. No references found.					
Formula: [REDACTED]			Eq Wt:		
Mol Weight: [REDACTED]		Wt% < 500: [REDACTED]		Wt% < 1000: [REDACTED]	
MP:		BP: 439		VP: <0.000001	
H2O Sol (g/L): 17.1 g/L, dispersible		Physical State: Liquid (est)		Log P: 0.53 [REDACTED]	
Endpoint (mg/L)	Est. Value	Meas. Value	Comments		
Fish 96-h	40				
Daphnid 48-h	40				
Algal 96-h	40				
Fish ChV	4.0				
Daphnid ChV	4.0				
Algal ChV	4.0				
BCF					
CHEMICAL CLASS:		SAR: Surf - non- [REDACTED]			
ECOTOX CONCERN	H	<input checked="" type="radio"/>	L	CONCERN CONCENTRATION	0.40
DATE 9/28/01		ASSESSOR:			

CHEMICAL: Unknown

10:20:15 09/27/:1

MOL WT :

MOL FOR:

SMILES :

ISOC-ID:

FRAG-ID:

H-COUNT:

Class

Type

Contribution Description

Comment

Value

RESULT

v3.3

All fragments measured

ESTIMATE

0.528

Press ENTER to continue...

OPPT STRUCTURE ACTIVITY TEAM (SAT) MEETING

DATE SEP 28 2001

ATTENDEES

SIGNATURE

CHEMISTRY

☒ Paul Bickart
☐ Diana Darling
☐ Rich Engler
☐ Greg Fritz
☐ Daniel Lin
☒ Kathy Schechter

Paul Bickart

Kathy Schechter

ENVIRONMENTAL FATE

☐ Bob Boethling
☐ David Lynch
☒ Gary Thom

gthom

HEALTH

☐ Katherine Anitole
☒ Michael Cimino
☒ Leonard Keifer
☐ David Lai
☐ Jim Murphy
☐ Deborah Norris
☐ Ronald Ward
☒ Yin Tak Woo

Michael Cimino
Leonard Keifer

Yin Tak Woo

ENVIRONMENTAL EFFECTS

☒ Gordon Cash
☐ Vince Nabholz
☐ Maggie Wilson

Gordon Cash

SAT CHAIRPERSON/OTHER

☐ Rebecca Jones
☐ Leonard Keifer
☒ Vince Nabholz

Vince Nabholz